

ON THE TOTAL NUMBER OF  
POLYHEXES WITH TEN HEXAGONS\*B. N. Cyvin, Zhang Fuji,<sup>\*\*</sup> Guo Xiaofeng,<sup>\*\*</sup>

J. Brunvoll and S. J. Cyvin

*Division of Physical Chemistry, The University of Trondheim,  
N-7034 Trondheim, Norway*

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*Abstract:* It is claimed that the total number of polyhexes with ten hexagons ( $h = 10$ ) has been given erroneously in the literature. The crucial problem is to enumerate correctly the non-Kekuléan helicenes (simply connected, geometrically nonplanar polyhexes) with  $h = 10$ . This task was solved by considering such systems with  $n_i = 5, 4, 3, 2$  and  $1$ , successively. Here  $n_i$  is used to designate the number of internal vertices. For  $n_i > 1$  the pertinent numbers were deduced by analytical methods of combinatorial enumerations (without computer aid). For  $n_i = 1$  the crucial number was obtained from a recently derived generating function for the simply connected polyhexes with  $n_i = 1$ , combined with a known number from the literature.

## 1. INTRODUCTION

"On the Total Number of Polyhexes" is the title of a paper [1] published in an earlier issue of Match. This paper or "mini-review" from the Düsseldorf-Zagreb group has given much inspiration to later works in the enumeration of polyhexes and is perhaps the

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\*\* On leave from: Department of Mathematics, Xinjiang University, Wulumuqi Xinjiang 830046, P.R. China.

most cited paper in a recent review on the topic [2]. The Düsseldorf–Zagreb group has also published many later papers on the enumeration of polyhexes, of which we cite a selection here [3–9]. These researchers have achieved excellent results in the enumeration of polyhexes and other chemical graphs [10]. Nevertheless we claim that they are not infallible. In particular, their total numbers for polyhexes with  $h > 7$  were found to be in error. Here  $h$  is the number of hexagons. These (wrong) numbers have been repeated in the monograph from the Düsseldorf–Zagreb group [10]. Corrections of the numbers for  $h = 8$  and  $h = 9$  are to be published elsewhere [11]. The corresponding number for  $h = 10$  has a more complicated history. In the original number, viz. 34350 [1,10], one helicirculene was omitted, as has been pointed out previously [2]. Hence the new number 34351 was launched [2]. In the meantime the Düsseldorf–Zagreb group claimed that the correct total number of polyhexes with  $h = 10$  should be 34347 [4], but in this number all helicirculenes were omitted. This wrong number has also been repeated elsewhere, by Trinajstić [12].

In the present paper we claim to have deduced the correct total number of polyhexes with  $h = 10$  for the first time. At the same time we exemplify two analytical methods of polyhex enumerations (without computer aid). Furthermore, we report the result of a mathematical solution for the numbers of a certain class of polyhexes.

## 2. CLASSES OF POLYHEXES WITH TEN HEXAGONS

The total number of polyhexes with  $h = 10$  is composed of the numbers for certain classes of polyhexes as specified in the following.

- (i) Simply connected, geometrically planar (non–helicenic) polyhexes: the benzenoids. This class is covered by the Düsseldorf–Zagreb numbers [1,10,13–15]. For  $h = 10$  the number is **30086**.
- (ii) Multiply connected, geometrically planar polyhexes: the planar circulenes. The Lunn numbers [16] pertain to all geometrically planar polyhexes. Hence the numbers of planar circulenes are obtained on subtracting the Düsseldorf–Zagreb numbers from them; for  $h = 10$ :  $30490 - 30086 = 404$ . The same number was produced independently by the Düsseldorf–Zagreb group [15]. This number contains one dicirculene with two holes, each of the size of one hexagon, in spite of the statement given elsewhere [1,10] that it only contains monocirculenes. The coronoids, which by definition contain holes of the sizes of at least two hexagons, form a subclass of the planar circulenes and are therefore counted already. For  $h = 10$  the 43 [4] single coronoids (one hole each) represent the whole set of coronoids with this number of hexagons.
- (iii) Simply connected, geometrically non–planar (helicenic) polyhexes: the helicenenes. The Düsseldorf–Zagreb group reported [1,10] 3857 helicenenes with  $h =$

10, of which 2736 were claimed to be pericondensed. A pericondensed polyhex is defined by having  $n_i > 0$ , in contrast to a catacondensed polyhex with  $n_i = 0$ . Here  $n_i$  is the number of internal vertices. The enumeration of helicenes with  $h = 10$  is the main subject of the present work since we claim that the two numbers [1,10] given above are wrong. We shall find it expedient to divide this class into some subclasses as follows. (a) Catacondensed helicenes. For  $h = 10$  this subclass contains 1121 systems [1,10]. The number emerges as the difference between a Harary-Read number [17] for catacondensed simply connected polyhexes and a number for the catacondensed, simply connected and geometrically planar polyhexes (catacondensed benzenoids) supplied by the Düsseldorf-Zagreb group [1,10,13,14]: 6693 - 5572. (b) Pericondensed Kekuléan helicenes. A Kekuléan polyhex has by definition  $K > 0$  in contrast to a non-Kekuléan polyhex with  $K = 0$ . Here  $K$  is the number of Kekulé structures. The subclass in question counts 797 systems, as can be extracted from the computerized enumerations of Herndon [18]. This number was confirmed by an analytical enumeration (without computer aid) [19]. (c) Pericondensed non-Kekuléan helicenes. This subclass for  $h = 10$  is enumerated for the first time in the present work.

- (iv) Multiply connected, geometrically non-planar polyhexes: Helicirculenes; 4 systems with  $h = 10$  [2].

In conclusion we find that it is necessary to derive the number of pericondensed non-Kekuléan helicenes with  $h = 10$  in order to attain at the correct total number of polyhexes for this number of hexagons. It is convenient to divide this task according to a further subdivision of the systems with respect to their numbers of internal vertices.

For helicenes with a given  $h$  it was found [11,20]

$$0 \leq n_i \leq 2h - 3 - \lceil (12h + 9)^{1/2} \rceil \quad (1)$$

where the "ceiling" function is employed;  $\lceil x \rceil$  is the smallest integer larger than or equal to  $x$ . The upper and lower bounds in the above equation, as well as all the intermediate integer values for  $n_i$  are always realized in helicenes. For non-Kekuléan helicenes the same  $n_i$  values except  $n_i = 0$  are realized. Accordingly, the cases to be considered for the pericondensed non-Kekuléan helicenes with  $h = 10$  are  $n_i = 1, 2, 3, 4, 5$ . For the sake of convenience the pericondensed helicenes are referred to as perihelicenes in the following.

### 3. PERIHELICENES WITH FIVE INTERNAL VERTICES

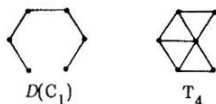
Polyhexes with  $n_i = 5$ , an odd number, are all non-Kekuléan. Two analytical methods were applied to the case of  $h = 10$ ,  $n_i = 5$  for perihelicenes.

**3.1. Combinatorial Enumeration.** An analytical method (without using computers), referred to as combinatorial enumeration, has been developed and applied previously to

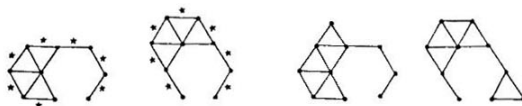
perihelicenes with  $h = 8$  and 9 [21] and to Kekuléan perihelicenes with  $h = 10$  [19].

The method is based on additions to irreducible helicenes in order to generate the desired helicenes  $H$ . An irreducible helicene,  $H^*$ , is a helicene which is no longer a helicene when any of its hexagons are deleted. A system  $H$  should always be deduced from a smallest possible  $H^*$ . It is convenient to employ the dualist [2,8,22] representation in this method. The dualist of a helicene  $H$  is identified by the symbol  $D(H)$ .

An application to the case of  $h = 10$ ,  $n_2 = 5$  is very simple. Firstly, it is found by methods which have been described in detail elsewhere [19,20], that  $H^* = C_1$  is the only possibility, where  $C_1$  is hexahelicene (see the below diagram). Secondly,  $H$  must contain benzo[ghi]perylene as a subgraph, of which the dualist is identified by  $T_4$ :



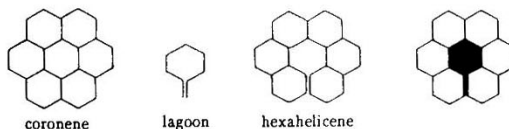
Furthermore, it is clear that  $T_4$  must be added to  $D(C_1)$  so that it shares two edges with it. The dualist of the resulting system is designated  $D(C_1) + T_4$ . Then it remains to add one triangle to  $D(C_1) + T_4$  so that it shares one edge with it. There are two nonisomorphic  $D(C_1) + T_4$  systems with  $h = 9$  each [21]. The last triangle can be attached to one of the seven edges in each case as indicated by the asterisks:



The above diagram includes two of the 14 nonisomorphic  $D(H)$  systems. Notice that, in a dualist  $D(H)$ , the vertices represent the hexagons of  $H$ , while the triangles in  $D(H)$  represent the internal vertices of  $H$ .

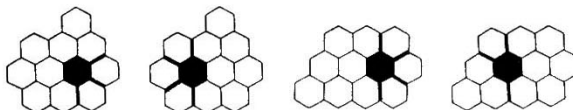
**3.2. Introduction of Lagoons.** Another combinatorial method for enumeration of helicenes shall presently be referred to as the introduction of "lagoons" [20]. The method is generally applicable to extremal helicenes, which are defined by having the maximum number of internal vertices for a given  $h$ ;  $n_i = (n_i)_{\max}$ . The values of  $(n_i)_{\max}$ , as a function of  $h$ , are given by the upper bound of eqn. (1).

In the below diagram hexahelicene is generated by introducing a lagoon in coronene.



Coronene is an extremal benzenoid [20,23,24], viz. a benzenoid with the maximum number of internal vertices (here six) for a given number of hexagons (here seven). It is emphasized that the term benzenoid is used here in the sense of simply connected, geometrically planar polyhex (which may be Kekuléan or non-Kekuléan). By introducing a lagoon as indicated above, the number of hexagons is lowered by one, while the number of internal vertices is lowered by six. In this special case the unique extremal helicene with  $h = 6$ ,  $n_i = 0$  is generated from the unique extremal benzenoid with  $h = 7$ ,  $n_i = 6$ . This is consistent with the long known fact that hexahelicene is the unique catacondensed helicene with six hexagons [22]. Now it is inferred that all the nonisomorphic extremal helicenes with  $h$  hexagons and  $n_i$  internal vertices are obtained by introducing a lagoon in all possible ways in everyone of the extremal benzenoids with  $h + 1$  hexagons and  $n_i + 6$  internal vertices.

The present case of  $h = 10$ ,  $n_i = 5$  deals with extremal helicenes. The extremal benzenoids of interest are those with eleven hexagons and eleven internal vertices. There are two nonisomorphic systems of this category [25]. Nonisomorphic helicenes can be generated by introducing lagoons in seven ways from each of these benzenoids. This feature is indicated below by black hexagons and heavy lines in the style as shown in the right-hand drawing of the above diagram.



The result, viz. fourteen helicenes with  $h = 10$ ,  $n_i = 5$ , is consistent with the result in Paragraph 3.1. Exactly the same systems are generated according to both methods (Paragraphs 3.1 and 3.2).

#### 4. NON-KEKULÉAN PERIHELICENES WITH FOUR INTERNAL VERTICES

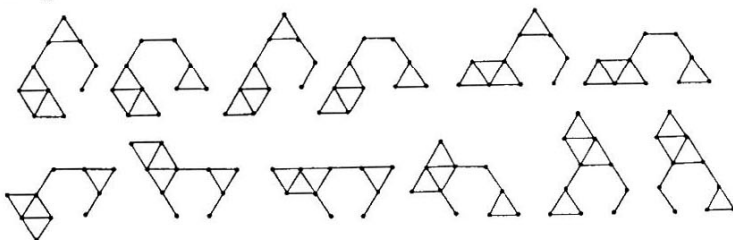
A polyhex with  $n_i = 4$ , an even number, is either Kekuléan or non-Kekuléan. The Kekuléan helicenes with  $h = 10$ ,  $n_i = 4$  have been enumerated elsewhere [19]. The

corresponding non-Kekuléan systems are treated in the following.

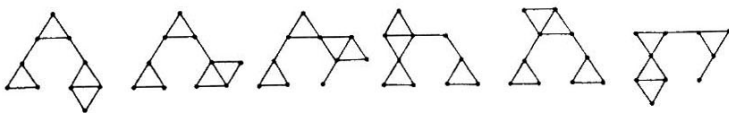
4.1. *Combinatorial Enumeration.* The analytical method of combinatorial enumeration (cf. Paragraph 3.1) was applied to the non-Kekuléan helicenes with  $h = 10$ ,  $n_i = 4$ . Exactly the same pattern could be used as in the case of the corresponding Kekuléan systems [19], with the exception of the addition of triangulene to hexahelicene, resulting in 1 system depicted below (as a dualist). Case (i):



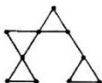
Also in all the other relevant cases,  $H^* = C_1$ . As Case (ii) take  $D(H)$  that contains the dualist of naphthanthrene ( $T_3$ ) and one separate triangle ( $T_1$ ). Both  $T_3$  and  $T_1$  must necessarily share an edge each with  $D(C_1)$ . In this way the following 12  $D(H)$  systems emerge.



Case (iii):  $D(H)$  contains the dualist of pyrene ( $T_2$ ) and two triangles; none of these should share an edge with  $T_2$ . The  $T_2$  unit and the two triangles not belonging to  $T_2$  must all share one edge each with  $D(C_1)$ . The following 6 systems of  $D(H)$  are generated.



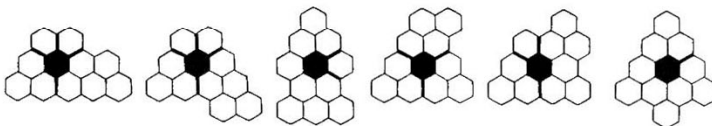
In Case (iv) the four triangles of  $D(H)$  have at most one common vertex. Only 1 system is possible:



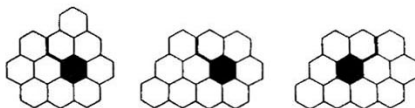
On addition of the numbers from Cases (i) – (iv) one obtains the result of 20 nonisomorphic non-Kekuléan helicenes with  $h = 10$ ,  $n_i = 4$ .

**4.2. Introduction of Lagoons.** The helicenes under consideration ( $h = 10$ ,  $n_i = 4$ ) are not extremal. Nevertheless, the method with introduction of lagoons can be applied in a slightly extended form.

Let a lagoon first be introduced as in the above example (Paragraph 3.2). Then we should look for the benzenoids with eleven hexagons and ten internal vertices. The forms of the twenty-six benzenoids of this category are known [25]. Out of these there are six non-Kekuléans, which are the ones of interest in the present analysis. They lead to 17 non-Kekuléan helicenes with  $h = 10$ ,  $n_i = 4$  as indicated below.



In order to obtain the remaining 3 systems we must introduce a "generalized lagoon" which removes one hexagon as before, but seven rather than six internal vertices. Then the initial benzenoids should have eleven hexagons and eleven internal vertices, the same as in the case of Paragraph 3.2. These benzenoids are non-Kekuléan, but the generalized lagoon (see below) creates Kekuléan helicenes in some positions and non-Kekuléan in others. The following three non-Kekuléan helicenes emerge from the analysis.

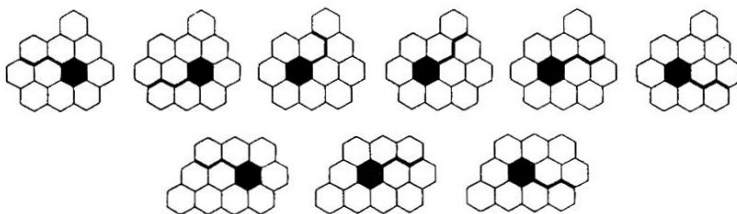


It is clear that the method with introduction of lagoons must be used with caution when the helicenes to be generated are not extremal. When the systems depart more and more from extremal helicenes (i.e.  $n_i$  decreases for given  $h$ ) then more and

more types of "generalized lagoons" must be taken into account. Furthermore, the method of introducing lagoons generates only helicenes with overlapping edges, but not with overlapping hexagons (e.g. heptahelicene).

## 5. PERIHELICENES WITH THREE INTERNAL VERTICES

In the case of the perihelicenes with  $h = 10$ ,  $n_i = 3$  (which all are non-Kekuléan) the method with introduction of (generalized) lagoons is impracticable. One would have to introduce the two types of lagoons which are found in Paragraph 4.2 into benzenoids with eleven hexagons having nine and ten internal vertices, respectively. There are exactly 100 systems of those with nine internal vertices [26,27] and 26 of those with ten [25,27]. As to the forms of these systems only the latter ones, viz. those with eleven hexagons and ten internal vertices, have been depicted [25]. In addition, a third type of generalized lagoons would have to be taken into account, one which decreases the number of hexagons by one and the number of internal vertices by eight. It should be introduced in the two benzenoids with eleven hexagons and eleven internal vertices, as indicated below.

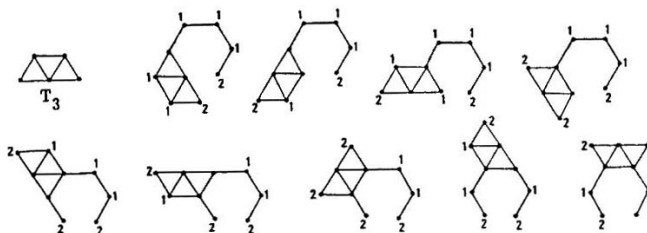


A full analysis of the systems under consideration according to the method of combinatorial enumeration (Paragraph 3.1), on the other hand, is very well feasible and is reported in the following.

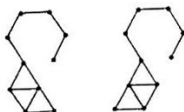
Three triangles (corresponding to three internal vertices) are to be added to an irreducible helicene,  $H^*$ . Then, for  $h = 10$ , it is clear that  $H^* = C_1$  (hexahelicene) in all cases. In this section  $H$  refers to a helicene with  $h = 10$ ,  $n_i = 3$ .

*Case 1.*  $D(H)$ , the dualist of  $H$ , contains  $T_3$ , the dualist of naphthanthrene. *Subcase 1.1.*  $T_3$  shares one edge with  $D(C_1)$ , and  $D(H)$  contains no subgraph  $D(C_6)$ , where  $C_6$  is heptahelicene. The  $D(H)$  systems are generated from the nine  $D(C_1) + T_3$  systems [21],

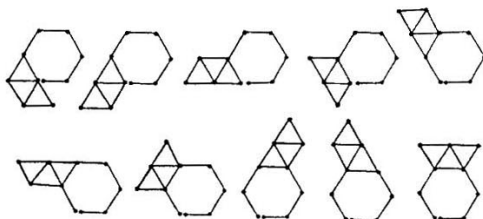
to which one edge should be attached, thus increasing the number of hexagons by one. The numerals in the below diagram indicate the numbers of ways an edge can be attached to the respective vertices. In the last case (the bottom-right figure) the symmetry must be taken into account. Symmetry considerations in order to avoid nonisomorphic systems are also made, without further mentioning, in several of the subsequent cases.



This gives 77 nonisomorphic  $D(H)$  systems. *Subcase 1.2.*  $T_3$  shares one vertex with  $D(C_1)$ , and  $D(H)$  contains no  $D(C_6)$ . The following 2 systems are generated.

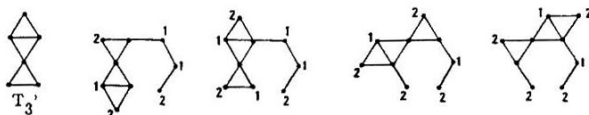


*Subcase 1.3.*  $D(H)$  contains  $D(C_6)$ . Then  $T_3$  must share one edge with  $D(C_6)$ , and the following 10 systems emerge.

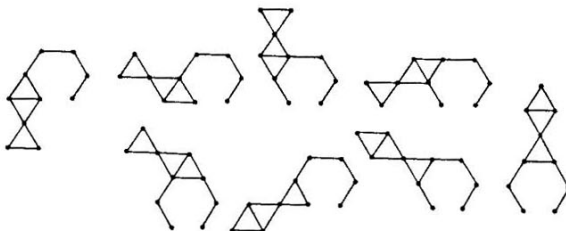


*Case 2.*  $D(H)$  contains  $T_3$ . *Subcase 2.1.*  $T_3$  shares two edges with  $D(C_1)$ , and  $D(H)$

contains no  $D(C_6)$ . The possibilities are indicated below as in Subcase 1.1.



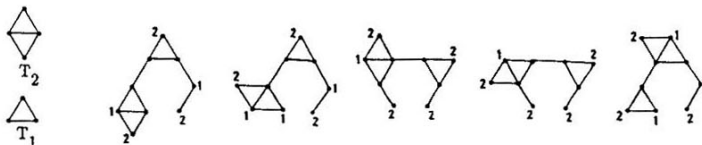
This gives 39 nonisomorphic  $D(H)$  systems. Subcase 2.2.  $T_3'$  shares one edge with  $D(C_1)$ , and  $D(H)$  contains no  $D(C_6)$ . The 8 possibilities are depicted below.

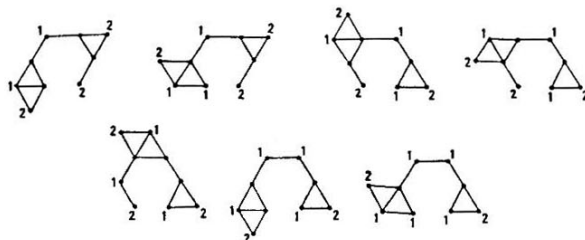


Subcase 2.3.  $D(H)$  contains  $D(C_6)$ . Then  $T_3'$  must share two edges with  $D(C_6)$ , and the following 5 systems are deduced.



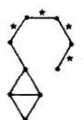
Case 3.  $D(H)$  contains  $T_2$ , the dualist of pyrene, and one triangle ( $T_1$ ) separated from each other. Subcase 3.1.  $T_2$  and  $T_1$  share one edge each with  $D(C_1)$ , and  $D(H)$  contains no  $D(C_6)$ . Again one more edge should be added to the system (as in Subcase 1.1), and the possibilities are specified below.



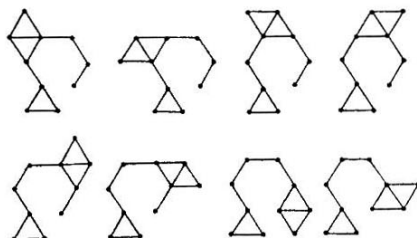


On adding the above numerals one arrives at 105 systems of  $D(H)$  under this subcase.

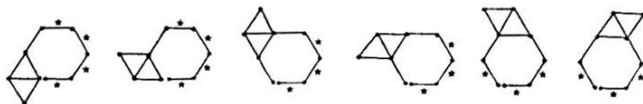
*Subcase 3.2.*  $T_2$  shares one vertex,  $T_1$  one edge with  $D(C_1)$ , and  $D(H)$  contains no  $D(C_6)$ . The 4 possibilities may be compressed in one figure, where the asterisks (as in Paragraph 3.1) indicate the positions for  $T_1$ ;



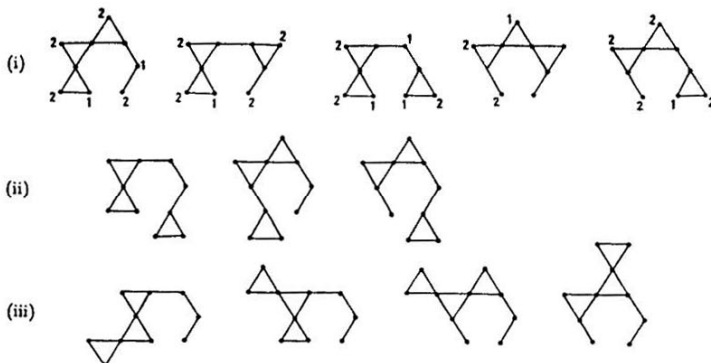
*Subcase 3.3.*  $T_1$  shares one vertex,  $T_2$  one edge with  $D(C_1)$ , and  $D(H)$  contains no  $D(C_6)$ . The following 8 systems emerge.



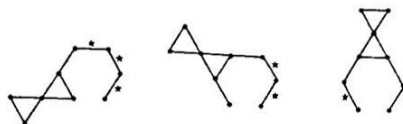
*Subcase 3.4.*  $D(H)$  contains  $D(C_6)$ . Then  $T_2$  and  $T_1$  must each share one edge with  $D(C_6)$ . Again let asterisks indicate the positions of  $T_1$ . Then the 20 possibilities may be mapped as in the following.



*Case 4.*  $D(H)$  contains  $T_2'$ , the dualist of perylene, and one triangle ( $T_1$ ) not sharing more than one vertex with  $T_2'$ . *Subcase 4.1.*  $T_2'$  shares two edges with  $D(C_1)$ , and  $D(H)$  contains no  $D(C_6)$ . Then  $T_1$  may share (i) one edge, (ii) one vertex or (iii) no vertex with  $D(C_1)$ . These possibilities, which lead to 42, 3 and 4  $D(H)$  systems, respectively, are specified in the following.



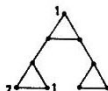
*Subcase 4.2.*  $T_2'$  shares one edge with  $D(C_1)$ . Then also  $T_1$  must share one edge with  $D(C_1)$ , and  $D(H)$  can not contain  $D(C_6)$ . The 6 possibilities are mapped below.



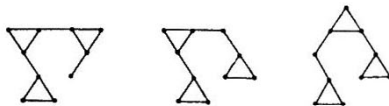
*Subcase 4.3.*  $D(H)$  contains  $D(C_6)$ . Then  $T_2'$  must share two edges and  $T_1$  one edge with  $D(C_6)$ . The 8 possibilities are indicated in the below diagram.



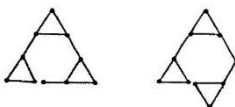
*Case 5.*  $D(H)$  contains three separate triangles. *Subcase 5.1.* All of the triangles share one edge each with  $D(C_1)$ , and  $D(H)$  contains no  $D(C_6)$ . The simple scheme



gives 4 systems  $D(H)$  as a result. *Subcase 5.2.* One triangle shares only one vertex with  $D(C_1)$ , and  $D(H)$  contains no  $D(C_6)$ . Then the other two triangles must share one edge each with  $D(C_1)$ , and 3 systems emerge:



*Subcase 5.3.*  $D(H)$  contains  $D(C_6)$ . Then the three triangles must share one edge each with  $D(C_6)$ , and one obtains the following 2 systems.



*Conclusion.* On adding the appropriate numbers of the above analysis it is concluded that there are 350 nonisomorphic helicenes with  $h = 10$ ,  $n_i = 3$ .

## 6. NON-KEKULÉAN PERIHELICENES WITH TWO INTERNAL VERTICES

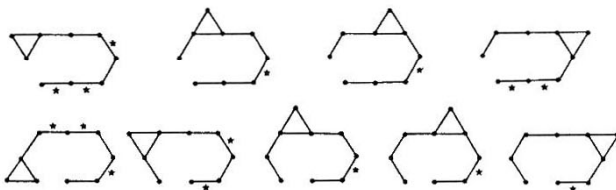
For the non-Kekuléan perihelicenes with  $h = 10$ ,  $n_i = 2$ , again a full analysis with introduction of lagoons is impracticable. However, a part of the problem can be solved by means of a new type of generalized lagoons, one which decreases the number of hexagons by two and the number of internal vertices by ten. The initial benzenoids are those which possess twelve hexagons and twelve internal vertices. Only the

non-Kekuléan benzenoids of this category are of interest, and their number is only three [25]. The below diagram indicates the fifteen helicenes deduced in the way as described above.



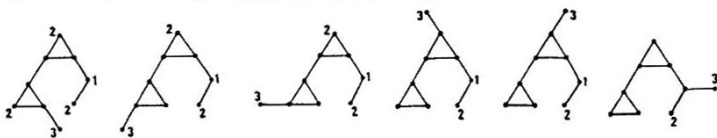
A full analysis of the systems under consideration by the combinatorial enumeration, on the other hand, was performed without much difficulties. It is reported in the following.

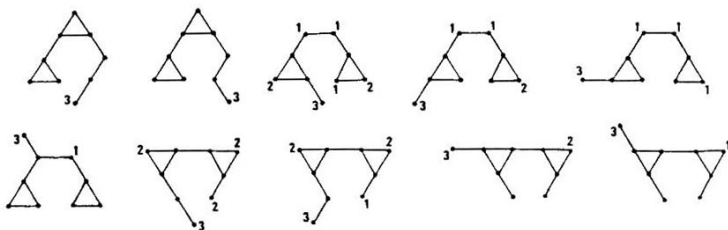
*Case A.* The initial irreducible helicene may be one of the  $h = 8$  systems  $C_2$  or  $C_3$  [21]. Assume as the first case that  $H^* = C_2$  or  $C_3$ . Then two triangles are to be added to  $D(C_2)$  or  $D(C_3)$ , and each of them must share one edge with the dualist of the respective irreducible helicene. The resulting 15 systems are identical with those of the above description and are contained in the below diagram.



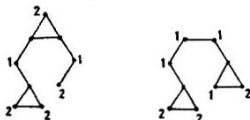
Here again each asterisk indicates the attachment of one triangle. Notice that the two triangles in each system must point in the opposite directions (upwards and downwards) in order to avoid the Kekuléans.

*Case B.*  $H^* = C_1$ . Two triangles are to be added to  $D(C_1)$ . *Subcase B1.* The two triangles share one edge each with  $D(C_1)$ , and  $D(H)$  contains no  $D(C_6)$ . Then two more edges are to be added to the dualist which has emerged. In the below mapping one added edge is drawn, while the possibilities for the other edge are indicated by numerals.

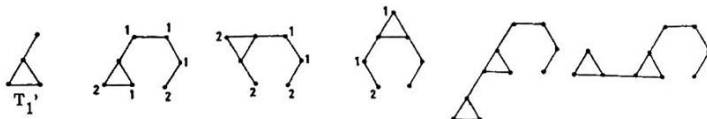




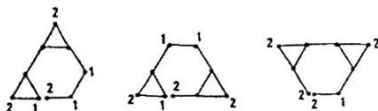
On adding all the numerals in the above diagram one arrives at 102 systems  $D(H)$ . *Subcase B2.* One triangle shares an edge and the other only one vertex with  $D(C_1)$ , while  $D(H)$  contains no  $D(C_6)$ . The below diagram should now be selfexplanatory.



As a result one obtains 20 systems under this subcase. *Subcase B3.* One triangle shares an edge with  $D(C_1)$ , while the conformation  $T_1'$  (see below) is attached by the vertex of degree one to  $D(C_1)$ . The numbers of possibilities for such attachments are indicated by numerals in the below diagram. For the sake of clarity also two complete systems are drawn.

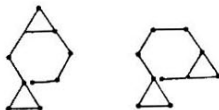


Under this subcase we count 20 systems. *Subcase B4.*  $D(H)$  contains  $D(C_6)$ , and the two triangles share one edge each with  $D(C_6)$ . It is also assumed that  $D(H)$  does not contain the subgraph  $D(C_7)$ , which makes it fall under a subsequent subcase. Now the following scheme is deduced.

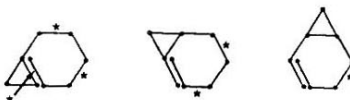


It gives 27 systems  $D(H)$ . *Subcase B5.*  $D(H)$  contains  $D(C_6)$ , and one of the triangles

should share only one vertex with  $D(C_6)$ . Then the other triangle must share an edge with  $D(C_6)$ , and the following 2 systems emerge.



*Subcase B6.*  $D(H)$  contains  $D(C_7)$ , the dualist of octahelicene. Then the two triangles must share one edge each with  $D(C_7)$ , and 6 nonisomorphic  $D(H)$  systems are deduced as indicated below.



*Conclusion.* From the above analysis it is concluded that there are 192 nonisomorphic non-Kekuléan helicenes with  $h = 10$ ,  $n_i = 2$ .

## 7. PERIHELICENES WITH ONE INTERNAL VERTEX

An enumeration of the perihelicenes with  $h = 10$ ,  $n_i = 1$ , which count more than thousand systems, is feasible, but on the limit where such an analysis can be performed correctly with confidence.

Therefore it is fortunate that a general mathematical solution recently has been achieved for the numbers of simply connected polyhexes with  $n_i = 1$  [28]. A generating function was derived in the style of the Harary-Read [17] generating function for the catacondensed simply connected polyhexes. Let the number of the (pericondensed) simply connected polyhexes with  $h$  hexagons and  $n_i = 1$  be identified by the symbol  $P_h$ . Then [28]

$$\begin{aligned} & \frac{1}{2}(2-9x+21x^2-16x^3) - \frac{1}{6}(4-18x+17x^2)(1-x)^{1/2}(1-5x)^{1/2} \\ & - \frac{1}{2}x(1-x^2)^{1/2}(1-5x^2)^{1/2} - \frac{1}{3}(1-x^3)^{1/2}(1-5x^3)^{1/2} \\ & = \sum_{i=1}^{\infty} P_i x^i = x^3 + x^4 + 6x^5 + 24x^6 + 109x^7 + 477x^8 \\ & \quad + 2155x^9 + 9647x^{10} + 43621x^{11} + 197767x^{12} + \dots \end{aligned}$$

The number of interest in the present work is the coefficient of  $x^{10}$ , viz. 9647, the number of nonisomorphic simply connected polyhexes with  $h = 10$ ,  $n_i = 1$ .

The number of simply connected, geometrically planar polyhexes (benzenoids) with  $h = 10$ ,  $n_i = 1$  is well known from computer-generations [10,13]: 8395. Then the number of nonisomorphic helicenes with  $h = 10$ ,  $n_i = 1$  is obtained as the difference  $9647 - 8395 = 1252$ .

## 8. SUMMARY: NUMERICAL RESULTS

The resulting numbers (given in bold) from Sections 3 – 7 are also found in Table 1 and add up to a total of **1840** nonisomorphic non-Kekuléan helicenes with  $h = 10$ . Table 1 shows further details for the numbers of helicenes with  $h = 10$ , both Kekuléan (data from literature) and non-Kekuléan. Notice that an enumeration of a class of polyhexes with a given pair of invariants  $(h, n_i)$  at the same time is an enumeration of the corresponding (chemical) isomers  $C_n H_s$ .

Table 2 shows a gross survey of the numbers of helicenes. It corrects the corresponding table in the recent review, which was referred to in Introduction ("Table 8" [2]), and also some of the other errors discussed therein.

Another table from the review [2], viz. "Table 7", needs a revision for  $h \geq 8$ . It is provided by Table 3.

Table 1. Numbers of helicenes (simply connected, geometrically nonplanar polyhexes) with 10 hexagons.

$h$	$n_i$	Formula	Kekuléan	non-Kekuléan	Total
10	0	$C_{42}H_{24}$	1121 <sup>a</sup>	0	1121 <sup>a</sup>
	1	$C_{41}H_{23}$	0	1252 <sup>b</sup>	1252 <sup>b</sup>
	2	$C_{40}H_{22}$	717 <sup>c,d</sup>	192	909
	3	$C_{39}H_{21}$	0	350	350
	4	$C_{38}H_{20}$	80 <sup>c,d</sup>	20 <sup>c</sup>	100 <sup>c</sup>
	5	$C_{37}H_{19}$	0	14 <sup>c</sup>	14 <sup>c</sup>

<sup>a</sup> Knop, Szymanski, Jeričević and Trinajstić (1984)[1]; <sup>b</sup> Cyvin, Zhang and Brunvoll (1992) [28]. <sup>c</sup> Cyvin, Guo, Cyvin and Zhang (1992)[11]; <sup>d</sup> Zhang, Guo, Cyvin and Cyvin [19].

Table 2. Numbers of helicenes

<i>h</i>	Catacondensed	Pericondensed	Total
6	1 <sup>a</sup>	0	1 <sup>b</sup>
7	5 <sup>b</sup>	3 <sup>b</sup>	8 <sup>b</sup>
8	35 <sup>b</sup>	35 <sup>c,d</sup>	70 <sup>c</sup>
9	200 <sup>b</sup>	331 <sup>c,d</sup>	531 <sup>c</sup>
10	1121 <sup>b</sup>	2625	3746
11	5919 <sup>e</sup>	†	†
12	30509 <sup>e</sup>	†	†
13	153187 <sup>e</sup>	†	†
14	756825 <sup>e</sup>	†	†
15	3688195 <sup>e</sup>	†	†

<sup>a</sup> Balaban and Harary (1968) [22]; <sup>b</sup> Knop, Szymanski, Jeričević and Trinajstić (1984) [1];

<sup>c</sup> Cyvin, Guo, Cyvin and Zhang (1992)[11]; <sup>d</sup> Guo, Zhang, Cyvin and Cyvin [21];

<sup>e</sup> Cyvin, Brunvoll and Cyvin (1992) [2]. † Unknown.

Table 3. Numbers of simply connected polyhexes (benzenoids + helicenes)

<i>h</i>	Catacondensed	Pericondensed	Total
1	1 <sup>a</sup>	0	1 <sup>b</sup>
2	1 <sup>a</sup>	0	1 <sup>b</sup>
3	2 <sup>a</sup>	1 <sup>a</sup>	3 <sup>b</sup>
4	5 <sup>a</sup>	2 <sup>a</sup>	7 <sup>b</sup>
5	12 <sup>a</sup>	10 <sup>a</sup>	22 <sup>b</sup>
6	37 <sup>a</sup>	45 <sup>a</sup>	82 <sup>b</sup>
7	123 <sup>c</sup>	216 <sup>b</sup>	339 <sup>b</sup>
8	446 <sup>c</sup>	1059	1505
9	1689 <sup>d</sup>	5347	7036
10	6693 <sup>d</sup>	27139	33832
11	27034 <sup>d</sup>	†	†
12	111630 <sup>d</sup>	†	†

<sup>a</sup> Balaban and Harary (1968) [22]; <sup>b</sup> Cyvin, Brunvoll and Cyvin (1992) [2];

<sup>c</sup> Balaban (1969) [29]; <sup>d</sup> Harary and Read (1970) [17]. † Unknown.

Table 4. Numbers of polyhexes in total

$h$	Catacondensed	Pericondensed	Grand total
1	1 <sup>a</sup>	0	1 <sup>b</sup>
2	1 <sup>a</sup>	0	1 <sup>b</sup>
3	2 <sup>a</sup>	1 <sup>a</sup>	3 <sup>b</sup>
4	5 <sup>a</sup>	2 <sup>a</sup>	7 <sup>b</sup>
5	12 <sup>a</sup>	10 <sup>a</sup>	22 <sup>b</sup>
6	38 <sup>a</sup>	45 <sup>a</sup>	83 <sup>b</sup>
7	124 <sup>a</sup>	217 <sup>a</sup>	341 <sup>c</sup>
8	452 <sup>a</sup>	1066	1518 <sup>d</sup>
9	1709 <sup>a</sup>	5394	7103 <sup>d</sup>
10	6790 <sup>a</sup>	27450	34240

<sup>a</sup> Cyvin, Brunvoll and Cyvin [2]; <sup>b</sup> Klarner (1965) [30];

<sup>c</sup> Knop, Szymanski, Jeričević and Trinajstić (1984) [1];

<sup>d</sup> Cyvin, Guo, Cyvin and Zhang (1992)[11].

Finally we have the total numbers of polyhexes, which have been given erroneously for  $h \geq 8$  in "Table 9" of the mentioned review [2] and elsewhere (cf. Introduction). Table 4 gives, for the first time, the corrected total numbers of polyhexes for  $h \leq 10$ .

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